Heisenberg uncertainty principle for thermal response of the microtubules excited by ultra-short laser pulses

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Abstract

In this paper the heat signaling in microtubules (MT) is investigated. It is argued that for the description of the heat signaling phenomena in MT, the hyperbolic heat transport (HHT) equation must be used. It is shown that HHT is the Klein-Gordon (K-G) equation. The general solution for the K-G equation for MT is obtained. For the undistorted signal propagation in MT the Heisenberg uncertainty principle is formulated and discussed.

Key words: Microtubules; Heat signaling; Klein-Gordon equation; Heisenberg principle.

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1 Introduction

The aim of this paper is to provide a semi-quantum theory of intracellular heat transport of cell organelles and vesicles here termed “particles”. Numerous experimental studies have established that this particles are equipped with bound motor proteins which move them along microtubules and actin filaments [1]. For example anterograde transport of particles along microtubules in nerve axons is mediated by the motor protein kinesin [2]. In this system the motion of particles is not continuous but saltatory [3]: particles are transported for distances of typically ~ 10 nm at a more or less steady velocity of $\sim 1\mu\mathrm{ms}^{-1}$ but there are pauses lasting for upward of 1 s in which given particle is apparently undergoing Brownian motion and has presumably detached from the microtubule or is stuck.

Recently D. A. Smith and R. M. Simmons [4] developed the reaction – diffusion model for the motor assisted transport of intracellular particles. In this paper we propose the model for signaling phenomena inside the microtubules. Considering our results collected in the monograph [5] we argue that the transport phenomena *inside* the microtubules must be discussed in the frame of the *quantum* transport equations for the diameter of the microtubules is of the order of nanometers, i.e. the order of the molecules. In the paper we develop the Klein-Gordon (K-G) type transport equation and will obtain the solution of K-G for Cauchy boundary conditions.

Recently [10] the study of the motion of the kinesin motor along microtubules using *interference total internal reflection microscopy* was undertaken. This technique bears some similarity to earlier ones designed to study the proximal hydrodynamics behavior of polymers to a surface. The laser source wavelength currently used in the experiment is 532 nm. The two laser beams identical in divergence, intensity phase and polarization are obtained using a flat beam splitter. From experiment [10] the value of the diffusion coefficient of the bead along the microtubule is obtained, $D = 315\mathrm{nm}^2\mathrm{s}^{-1}$.

In this paper we study the heat signaling phenomena inside the microtubule excited by ultra-short laser pulses.

2 Heat pulse transport on the molecular scale

Molecular electronics is a new field of science and technology, which is evolving from the convergence of ideas from chemistry, physics, biology, electronics

and information technology. It considers, on the one hand molecular materials for electronic/optoelectronic applications, on the other hand attempts to build electronics with molecules at the molecular level. It is this second viewpoint which concerns us here: describing the heat transport at the level of single or few molecules.

The heat and charge transport phenomena on the molecular scale are the quantum phenomena and electrons constitute the charge and heat carriers. We argue, that to describe the heat transport phenomena on the molecular level the quantum heat transport equation is a natural reference equation. The quantum heat transport equation for the atomic scale has the form

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = D \nabla^2 T, \tag{1}$$

where τ is the relaxation time, D is the heat diffusion coefficient and T denotes temperature. For the atomic scale heat transport, the relaxation time equals

$$\tau = \frac{\hbar}{m v_h^2}, \qquad v_h = \frac{1}{\sqrt{3}} \alpha c, \tag{2}$$

where m is the electron mass and v_h is the velocity of the heat perturbation. Moreover, on the atomic level the temperature field $T(r)$ is quantized by a quantum heat of energy, the *heaton*. The *heaton* energy equals

$$E_h = m_e v_h^2. \tag{3}$$

Due to formula (3), the *heaton* energy is the interaction energy of electromagnetic field with electrons (through the coupling constant α).

At the molecular level we seek energy of interactions of the electromagnetic field with a molecule. This energy is described by the formula

$$E_h^m = \alpha^2 \frac{m_e}{m_p} m_e c^2, \tag{4}$$

where m_e, m_p are the masses of electron and proton, respectively.

Considering the general formula for *heaton* energy (3), one obtains from formula (4) for velocity of the thermal perturbation

$$v_h = \alpha c \left(\frac{m_e}{m_p} \right)^{1/2}. \tag{5}$$

Comparison of formulas (2) and (5) shows, that v_h scales with ratio $(m_e/m_p)^{1/2}$ when the atomic scale is changed to the molecular scale; v_h is the Fermi velocity for molecular gas.

Quantum heat transport equation (1) has as a solution, for short time scale, (short in comparison to relaxation time τ) the heat waves which propagate with velocity v_h. One can say that on the molecular level, the heat waves are slower in comparison to the atomic scale.

From formulas (2) and (5), the relaxation time can be calculated

$$\tau = \frac{m_p}{m_e} \frac{\hbar}{m_e c^2 \alpha^2}. \tag{6}$$

It occurs, that relaxation time on the molecular scale is longer (ratio m_p/m_e) than the atomic relaxation time. For standard values of the constants of the Nature

$$\alpha = \frac{1}{137}, \qquad m_e = 0.511\,\mathrm{MeV/c^2}, \qquad m_p = 938\,\mathrm{MeV/c^2}, \tag{7}$$

one obtains the following numerical values for v_h, τ and E_h: $v_h = 0.05\,\mathrm{nm/fs}$, $\tau = 44\,\mathrm{fs}$ and $E_h = 10^{-2}$ eV. With those values of v_h and τ, the mean free path

$$\lambda = \tau v_h \tag{8}$$

can be calculated and $\lambda = 2.26\,\mathrm{nm}$. It is interesting to observe, that in the structure of the biological cells (e.g. microtubules), some elements have the dimension of the order of the nanometer (e.g. microtubules).

With the help of the *heaton* energy one can define the *heaton temperature*, i.e., the characteristic temperature of the heat transport on the molecular scale, viz.:

$$T_m = \alpha^2 \frac{m_e}{m_p} m_e c^2 \, 1.16\, 10^{10}\,\mathrm{K} \approx 10^{-3} \alpha^2 m_e c^2 \sim 316\,\mathrm{K}. \tag{9}$$

This defines what we generally term “room temperature”. At temperatures far below T_m, the hydrogen bond becomes very rigid and the flexibility of atomic configurations is weakened. Most substances are liquid or solid below T_m. Biology occurs in environments with ambient temperature within an order or magnitude or so of T_m.

In the following we assume that the ambient temperature T_m is the initial temperature of the nerve cells.

Figure 1: (a) The solution of QHT equation (1) for the following input parameters $v_h = 5\ 10^{-2}\,\mathrm{nm/fs}, \tau = 44\,\mathrm{fs}, T_0 = 300\,\mathrm{K}$ and $\Delta t = 0.2\tau$. (b) The solution of QPT (11) with the same input parameters.

Figure 2: (a, b) The same as in Fig. 1(a, b) but for $\Delta t = \tau$.

In Figs. 1, 2 the results of the theoretical calculations for the quantum heat transport on the molecular scale are presented. In Fig. 1(a) the solution of Eq. (1) in one-dimensional case

$$\tau\frac{\partial^2 T}{\partial t^2}+\frac{\partial T}{\partial t}=D\frac{\partial^2 T}{\partial x^2}, \tag{10}$$

for the following input parameters $v_h = 0.05$ nm/fs, $\tau = 44$ fs, $T_0 = 300$ K (initial temperature) and Δt duration of laser pulse $= 0.2\tau$ is presented.

In Fig. 1(b) the solution of quantum parabolic heat transport equation (QPT), (Fourier equation)

$$\frac{\partial T}{\partial t}=D\frac{\partial^2 T}{\partial x^2} \tag{11}$$

with the same input parameters is presented.

In Figs. 2(a, b), the solutions of Eqs. (1), (11) for the same input parameter but for $\Delta t = \tau$ are presented.

From the analysis of the solutions of hyperbolic and parabolic quantum heat transport equation, the following conclusions can be drawn. In the case of QHT equation the thermal wave dominates the heat transport for $\Delta t = 0.2\,\tau$. The finite value of v_h involves the delay time for the response of the molecular system on the initial temperature change. In the case of QPT, instantaneous diffusion heat transport is observed. From the technological point of view, the strong localization of thermal energy in the front of thermal wave is very important.

3 Electron thermal relaxation in microtubules

Clusters and aggregates of atoms in the nanometer size (currently called nanoparticles) are systems intermediate in several respects, between simple molecules and bulk materials and have been objects of intensive work.

In this paper, we investigate the thermal relaxation phenomena in the nanoparticles - microtubules in the frame of quantum heat transport equation. In the book [5], the thermal inertia of materials heated with laser pulses faster than the characteristic relaxation time was investigated. It was shown, that in the case of the ultra-short laser pulses the hyperbolic heat conduction (HHC) must be used. For microtubules the diameters are of the order of the

electron de Broglie wave length. In that case to description of the transport phenomena quantum heat transport must be used [5].

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \frac{\hbar}{m} \nabla^2 T, \tag{12}$$

where T denotes the temperature of the heat carrier, τ is the relaxation time and m denotes the mass of heat carrier. The relaxation time τ is defined as [5]

$$\tau = \frac{\hbar}{m v_h^2}, \tag{13}$$

where v_h is the thermal pulse propagation velocity

$$v_h = \frac{1}{\sqrt{3}} \alpha c. \tag{14}$$

In formula (14) α is the coupling constant (for electromagnetic interaction $\alpha = e^2/\hbar c$) and c denotes the light velocity in vacuum. Both parameters τ and v_h completely characterize the thermal energy transport on the atomic scale and can be named as "*atomic relaxation time*" and *"atomic" heat velocity*.

Both τ and v_h are build up from constant of Nature, α, c. Moreover, on the atomic scale there is no shorter time period than τ and smaller velocity build from constant of the Nature. In consequence, one can name τ and v_h as *elementary relaxation time* and *elementary velocity*, which characterize heat transport in the elementary building block of matter, the atom.

In the following, starting with elementary τ and v_h, we intend to describe thermal relaxation processes in microtubules which consist of the N parts (molecules) each with elementary τ and v_h. To that aim, we use the Pauli-Heisenberg inequality [5]

$$\Delta r \Delta p \geq N^{\frac{1}{3}} \hbar, \tag{15}$$

where r denotes characteristic dimension of the nanoparticle and p is the momentum of energy carriers. The Pauli-Heisenberg inequality expresses the basic property of the N-fermionic system. In fact, compared to the standard Heisenberg inequality

$$\Delta r \Delta p \geq \hbar, \tag{16}$$

we notice that, in this case the presence of the large number of identical fermions forces the system either to become spatially more extended for

fixed typical momentum dispension, or to increase its typical momentum dispension for a fixed typical spatial extension. We could also say that for a fermionic system in its ground state, the average energy per particle increases with the density of the system.

A picturesque way of interpreting the Pauli-Heisenberg inequality is to compare Eq. (15) with Eq. (16) and to think of the quantity on the right hand side of it as the *effective fermionic Planck constant*

$$h^f(N) = N^{\frac{1}{3}}\hbar. \tag{17}$$

We could also say that antisymmetrization, which typifies fermionic amplitudes amplifies those quantum effects which are affected by Heisenberg inequality.

According to formula (17), we recalculate the relaxation time τ, formula (13) and thermal velocity v_h, formula (14) for nanoparticle consisting N fermions

$$\hbar \to \hbar^f(N) = N^{\frac{1}{3}}\hbar \tag{18}$$

and obtain

$$v_h^f = \frac{e^2}{\hbar^f(N)} = \frac{1}{N^{\frac{1}{3}}}v_h, \tag{19}$$

$$\tau^f = \frac{\hbar^f}{m(v_h^f)^2} = N\tau. \tag{20}$$

Number N parts in nanoparticle (sphere with radius r) can be calculated according to the formula (we assume that density of nanoparticle does not differ too much from bulk material)

$$N = \frac{\frac{4\pi}{3}r^3\rho AZ}{\mu} \tag{21}$$

and for spherical with semiaxes a, b, c

$$N = \frac{\frac{4\pi}{3}abc\rho AZ}{\mu}, \tag{22}$$

where ρ is the density of the nanoparticle, A is the Avogardo number, μ is the molecular mass of particles in grams and Z is the number of the valence electrons.

With formulas (19) and (20), we calculated de Broglie wave length λ_B^f and mean free path λ_{mfp}^f for nanoparticles

$$\begin{aligned}\lambda_B^f &= \frac{\hbar^f}{mv_{th}^f} = N^{\frac{2}{3}}\lambda_B, &(23)\\ \lambda_{mfp}^f &= v_{th}^f\,\tau_{th}^f = N^{\frac{2}{3}}\lambda_{mfp}, &(24)\end{aligned}$$

where λ_B and λ_{mfp} denote the de Broglie wave length and mean free path for heat carriers in nanoparticles.

4 Quantum transport in microtubules

Microtubules are essential to cell functions. In neurons microtubules help and regulate synaptic activity responsible for learning and cognitive functions. While microtubules have traditionally been considered to be purely structural elements, recent evidence has revelated that mechanical, chemical and electrical signaling and communication function also exist, the result of microtubule interaction with membrane structures by linking proteins, ions and voltage fields respectively.

The characteristic dimensions of the microtubules, crystalline cylinder 10 nm in inner diameter are of the order of the de Broglie length for electrons in atoms.

When the characteristic length of the structure is of the order of the de Broglie wave length, then the signaling phenomena must be described within the quantum transport theory.

For quantum transport phenomena in microtubules we will apply the equation (1) with the relaxation time described by formula (2)

$$\tau = \frac{2\hbar}{mv^2} = \frac{\hbar}{E}.$$

The relaxation time is the decoherence time, i.e. time until collapse of the wave function occurs, when the transition classical $\rightarrow$ quantum phenomena is considered.

In the following we will consider the time τ for the atomic and multiatomic phenomena. As was shown in section 2 for atomic phenomena

$$\tau_a \sim 10^{-17}\ \mathrm{s} \tag{25}$$

and when we consider multiatomic transport phenomena, with N equal number of agregates involved in transport we have, formula (20)

$$\tau_N = N\tau_a. \tag{26}$$

The Penrose-Hameroff Orchestrated Objective Reduction (Orch OR) model [2] proposes that quantum superposition - computation occurs in nanotubule automata within brain neurons and glia. Tubulin subumits within microtubules act as qubits, switching between states on a nanosecond scale, governed by London forces in hydrophobic pockets. These oscillations are tuned and orchestrated by microtubule associated proteins (MAPs) providing a feedback loop between the biological system and the quantum state. These qubits interact computationally by nonlocal quantum entanglement, according to the Schrödinger equation with preconscious processing continuing until the threshold for objective reduction (OR) is reacted ($E = \frac{\hbar}{T}$). At that instant, collapse occurs, triggering a "moment of awareness" or a conscious event - an event that determines particular configurations of Planck scale experiential geometry and corresponding classical states of nanotubules automata that regulate synaptic and other neural functions. A sequence of such events could provide a forward flow of subjective time and stream of consciousness. Quantum states in nanotubules may link to those in nanotubules in other neurons and glia by tunnelling through gap functions, permitting extension of the quantum state through significant volumes of the brain.

Table 1:

Event	T [ms]	E	N number of aggregates	τ [ms]
Buddhist moment of awareness	13	$4 \cdot 10^{15}$ nucleons	10^{15}	10
Coherent 40Hz oscillations	25	$2 \cdot 10^{15}$	10^{15}	10
EEG alpha rhytm (8 to 12 Hz)	100	10^{14}	10^{14}	1
Libet's sensory threshold	500	10^{14}	10^{14}	1

From $E = \frac{\hbar}{T}$, the size and extension of Orch OR events that correlate with subjective or neurophysiological description of conscious events can be calcu-

lated. In Table 1 the calculated T (Penrose-Hameroff) and $\tau-$ formula (26) are presented [6].

5 Heisenberg uncertainty principle for thermal phenomena in microtubules

Efficient conversion of electromagnetic energy to particle energy is of fundamental importance in many areas of physics. The nature of intense, short pulse laser interactions with single atoms and solid targets has been subject of extensive experimental and theoretical investigation over the last 15 years. Recently, the interaction of femtosecond laser pulses with Xe clusters was investigated and strong X-ray emission and multi-keV electron generation were observed. Such experiments have become possible, owing to recently developed high peak power lasers which are based on chirped pulse amplification and are capable of producing focused light intensity of up to $10^{14} - 10^{19}\,\mathrm{Wcm}^{-2}$.

In intensely irradiated clusters e.g. microtubules, optically and collisionally ionized electrons undergo rapid collisional heating for short time (< 1ps) before the cluster disintegrates in the laser field. Charge separation of the hot electrons inevitably leads to a very fast expansion of the cluster ions. Both electrons and ions ultimately reach a velocity given by the speed of sound of the cluster plasma.

When the intense laser pulse interacts with atomic clusters ionization to very high charge states is observed. The high Coulomb field certainly influences the thermal processes in clusters. In the chapter, the new QHT equation is formulated in which the external — not only thermal forces are included. The solution of the new QHT for Cauchy boundary conditions will be derived. The condition for the distortionless propagations of the thermal wave will be formulated.

Now, we develop the generalized quantum heat transport equation which includes the potential term. In this way, we use the analogy between the Schrödinger equation and quantum heat transport equations. Let us consider, for the moment, the parabolic heat transport equation with the second derivative term omitted

$$\frac{\partial T}{\partial t} = \frac{\hbar}{m}\nabla^2 T. \tag{27}$$

When the real time $t \to \frac{it}{2}$ and $T \to \Psi$, Eq. (27) has the form of a free

Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi. \tag{28}$$

The complete Schrödinger equation has the form

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi, \tag{29}$$

where V denotes the potential energy. When we go back to real time $t \to -2it$ and $\Psi \to T$, the new parabolic quantum heat transport is obtained

$$\frac{\partial T}{\partial t} = \frac{\hbar}{m}\nabla^2 T - \frac{2V}{\hbar}T. \tag{30}$$

Equation (30) describes the quantum heat transport for $\Delta t > \tau$. For heat transport initiated by ultra-short laser pulses, when $\Delta t \leq \tau$ one obtains the generalized quantum hyperbolic heat transport equation

$$\tau\frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \frac{\hbar}{m}\nabla^2 T - \frac{2V}{\hbar}T. \tag{31}$$

Considering that $\tau = \hbar/mv^2$, Eq. (31) can be written as follows:

$$\frac{1}{v^2}\frac{\partial^2 T}{\partial t^2} + \frac{m}{\hbar}\frac{\partial T}{\partial t} + \frac{2Vm}{\hbar}T = \nabla^2 T. \tag{32}$$

Equation (32) describes the heat flow when apart from the temperature gradient, the potential energy V operates.

In the following, we consider the one-dimensional heat transfer phenomena, i.e.

$$\frac{1}{v^2}\frac{\partial^2 T}{\partial t^2} + \frac{m}{\hbar}\frac{\partial T}{\partial t} + \frac{2Vm}{\hbar}T = \frac{\partial^2 T}{\partial x^2}. \tag{33}$$

For quantum heat transfer equation (33), we seek solution in the form

$$T(x,t) = e^{-t/2\tau}u(x,t). \tag{34}$$

After substitution of Eq. (34) into Eq. (33), one obtains

$$\frac{1}{v^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + q\,u(x,t) = 0, \tag{35}$$

where

$$q = \frac{2Vm}{\hbar^2} - \left(\frac{mv}{2\hbar}\right)^2. \tag{36}$$

In the following, we will consider the constant potential energy $V = V_0$. The general solution of Eq. (35) for Cauchy boundary conditions,

$$u(x,0) = f(x), \qquad \left.\frac{\partial u(x,t)}{\partial t}\right|_{t=0} = F(x), \tag{37}$$

has the form [5]

$$u(x,t) = \frac{f(x-vt)+f(x+vt)}{2} + \frac{1}{2}\int_{x-vt}^{x+vt} \Phi(x,t,z)dz, \tag{38}$$

where

$$\begin{aligned}
\Phi(x,t,z) &= \frac{1}{v}F(z)J_0\left(\frac{b}{v}\sqrt{(z-x)^2-v^2t^2}\right) + btf(z)\frac{J_0'\left(\frac{b}{v}\sqrt{(z-x)^2-v^2t^2}\right)}{\sqrt{(z-x)^2-v^2t^2}}, \\
b &= \left(\frac{mv^2}{2\hbar}\right)^2 - \frac{2Vm}{\hbar^2}v^2
\end{aligned} \tag{39}$$

and $J_0(z)$ denotes the Bessel function of the first kind. Considering formulas (34), (35), (36) the solution of Eq. (33) describes the propagation of the distorted thermal quantum waves with characteristic lines $x = \pm vt$. We can define the distortionless thermal wave as the wave which preserves the shape in the field of the potential energy V_0. The condition for conserving the shape can be formulated as

$$q = \frac{2Vm}{\hbar^2} - \left(\frac{mv}{2\hbar}\right)^2. \tag{40}$$

When Eq. (40) holds, Eq. (35) has the form

$$\frac{\partial^2 u(x,t)}{\partial t^2} = v^2\frac{\partial^2 u}{\partial x^2}. \tag{41}$$

Equation (41) is the quantum wave equation with the solution (for Cauchy boundary conditions (37))

$$u(x,t) = \frac{f(x-vt)+f(x+vt)}{2} + \frac{1}{2v}\int_{x-vt}^{x+vt} F(z)dz. \tag{42}$$

It is quite interesting to observe, that condition (40) has an analog in the classical theory of the electrical transmission line. In the context of the

transmission of an electromagnetic field, the condition $q = 0$ describes the Heaviside distortionless line. Eq. (40) — the distortionless condition — can be written as

$$V_0 \tau \sim \hbar, \tag{43}$$

We can conclude, that in the presence of the potential energy V_0 one can observe the undisturbed quantum thermal wave only when *the Heisenberg uncertainty relation for thermal processes* (43) is fulfilled.

The generalized quantum heat transport equation (GQHT) (33) leads to the generalized Schrödinger equation. After the substitution $t \to it/2$, $T \to \Psi$ in Eq. (33), one obtains the generalized Schrödinger equation (GSE)

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi - 2\tau\hbar \frac{\partial^2 \Psi}{\partial t^2}. \tag{44}$$

Considering that $\tau = \hbar/mv^2 = \hbar/m\alpha^2 c^2$ ($\alpha = 1/137$ is the fine-structure constant for electromagnetic interactions) Eq. (44) can be written as

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi - \frac{2\hbar^2}{m\alpha^2 c^2} \frac{\partial^2 \Psi}{\partial t^2}. \tag{45}$$

One can conclude, that for time period $\Delta t < \hbar/m\alpha^2 c^2 \sim 10^{-17}$ s the description of quantum phenomena needs some revision. On the other hand, for $\Delta t > 10^{-17}$ in GSE the second derivative term can be omitted and as the result the SE is obtained, i.e.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi. \tag{46}$$

It is quite interesting to observe, that GSE was discussed also in the context of the sub-quantal phenomena.

Concluding, a study of the interactions of the attosecond laser pulses with matter can shed the light on the applicability of the SE to the study of the ultra-short sub-quantal phenomena.

The structure of the Eq. (35) depends on the sign of the parameter q. For quantum heat transport phenomena with electrons as the heat carriers parameter q is the function of potential barrier height (V_0) and velocity v. Considering that velocity v equals

$$v = \frac{1}{\sqrt{3}} \alpha c = 1.26 \, \frac{\text{nm}}{\text{fs}}, \tag{47}$$

Figure 3: Parameter q (formula (36)) as the function of the barrier height (eV).

parameter q can be calculated for typical barrier height $V_0 \geq 0$. In Fig. 3 the parameter q as the function of V_0 is calculated. For $q < 0$, i.e., when V_0 <1.25 eV, Eq. (35) is the *modified Klein-Gordon equation*.

For Cauchy initial condition

$$u(x,o) = f(x), \qquad \frac{\partial u(x,o)}{\partial t} = g(x), \tag{48}$$

the solution of the Eq. (35) has the form

$$\begin{aligned} u(x,t) &= \frac{f(x-vt)+f(x+vt)}{2} \\ &+ \frac{1}{2v}\int_{x-vt}^{x+vt} g(\zeta) I_0\left[\sqrt{-q(v^2t^2-(x-\zeta)^2)}\right] d\zeta \\ &+ \frac{(v\sqrt{-q})t}{2}\int_{x-vt}^{x+vt} f(\zeta)\frac{I_1\left[\sqrt{-q(v^2t^2-(x-\zeta)^2)}\right]}{\sqrt{v^2t^2-(x-\zeta)^2}} d\zeta. \end{aligned} \tag{49}$$

When $q > 0$ Eq. (35) is the *Klein-Gordon equation* (K-G) well known from application to elementary particle and nuclear physics.

For Cauchy initial condition (48), the solution of (K-G) equation can be written as

$$
\begin{aligned}
u(x,t) &= \frac{f(x-vt)+f(x+vt)}{2} \\
&+ \frac{1}{2v}\int_{x-vt}^{x+vt} g(\zeta) J_0\left[\sqrt{q(v^2t^2-(x-\zeta)^2)}\right] d\zeta \\
&- \frac{v\sqrt{q}t}{2}\int_{x-vt}^{x+vt} f(\zeta)\frac{J_0'\left[\sqrt{q(v^2t^2-(x-\zeta)^2)}\right]}{\sqrt{v^2t^2-(x-\zeta)^2}} d\zeta.
\end{aligned}
\tag{50}
$$

Both solutions (49) and (50) exhibit the domains of dependence and influence on *modified Klein-Gordon equation* and *Klein–Gordon equation*. These domains, which characterize the maximum speed at which thermal disturbance travel are determined by the principal parts of the given equation (i.e., the second derivative terms) and do not depend on the lower order terms. It can be concluded that these equation and the wave equation (for $m = 0$) have identical domains of dependence and influence.

6 Thermal wave packets induced by attosecond laser pulses

Equation (35) is the modified Klein-Gordon equation which can be written as

$$\bar{\Box} u - \left(\frac{mv}{2\hbar}\right)^2 u(x,t) = 0, \tag{51}$$

where d'Alembert operator $\bar{\Box}$ is equal

$$\bar{\Box} = \frac{1}{v^2}\frac{\partial}{\partial t^2} - \frac{\partial}{\partial x^2}. \tag{52}$$

The ordinary Klein-Gordon equation for the particle with mass m and velocity v is of the form [5]

$$\bar{\Box} u + \left(\frac{m_0}{2\hbar}\right)^2 u = 0. \tag{53}$$

Equation (51) can be split into its real and imaginary parts. Putting for $u(x,t)$

$$u(x,t) = \Re(t,x)\exp\left[\frac{i}{\hbar}S(t,x)\right]$$

one obtains

$$\eta^{ab}(\partial_a S)(\partial_b S) = \hbar^2 \frac{\bar{\Box}\Re}{\Re} - \left(\frac{mv}{2}\right)^2, \tag{54}$$

where

$$\eta_{ab} = \mathrm{diag}(1, -1, -1, -1), \qquad a, b = 1, 2, 3, 4.$$

We use Mackinnon's suggestion [6] therefore we look for solutions that satisfy the equation

$$\frac{\bar{\Box}\Re}{\Re} = \left(\frac{mv}{\sqrt{2}\hbar}\right)^2. \tag{55}$$

In this way Eq. (54) becomes

$$\eta^{ab}(\partial_a S)(\partial_b S) = m^2 v^2 = P_\mu P^\mu. \tag{56}$$

If the velocity v is constant, we have from (54)

$$S = -P^\mu P_\mu \tag{57}$$

and the de Broglie relation $P^v = \hbar K^v$ hold where K^v is the wave number and P^v is the classical relativistic four momentum, $P^v = \left(\frac{E}{v}\vec{p}\right)$. In paper [6] L. Mackinnon constructs a wave packet considering that a wave $\Phi = \Phi_0 \exp\left[i\omega t\right]$ of frequency $\omega = \frac{mc^2}{\hbar}$ is associated with a particle of rest mass m and that for an observer moving with a constant velocity v with respect to the particle, the associated wave (be means of a Lorentz transformation) acquires the form $\Phi = \Phi_0 \exp\left[i\omega\gamma\left(t - \frac{v}{c^2}x\right)\right]$. Mackinnon showed the wave packet is compatible with the basic experiments of quantum mechanics and does not spread in time the found

$$\Re = A\frac{\sin[gr]}{gr}, \tag{58}$$

where $A =$ constant and $g = \frac{mv}{\sqrt{2}\hbar}$, and $g = \frac{m\alpha c}{\sqrt{2}\hbar}$ and

$$r = \gamma(x - vt) \tag{59}$$

is the distance from the particle portion, so that

$$u(x,t) = A\frac{\sin gr}{gr}\exp\left[-\frac{i}{\hbar}(Et - px)\right] \tag{60}$$

is the Lorentz boost of the solution

$$\Phi = A \frac{\sin g r'}{g r'} \exp\left[-i\omega t'\right],$$

where $r' = x$. This solution was first found by de Broglie [8] and also used in the stochastic interpretation of quantum mechanics by Vigier and Gueret [9].

References

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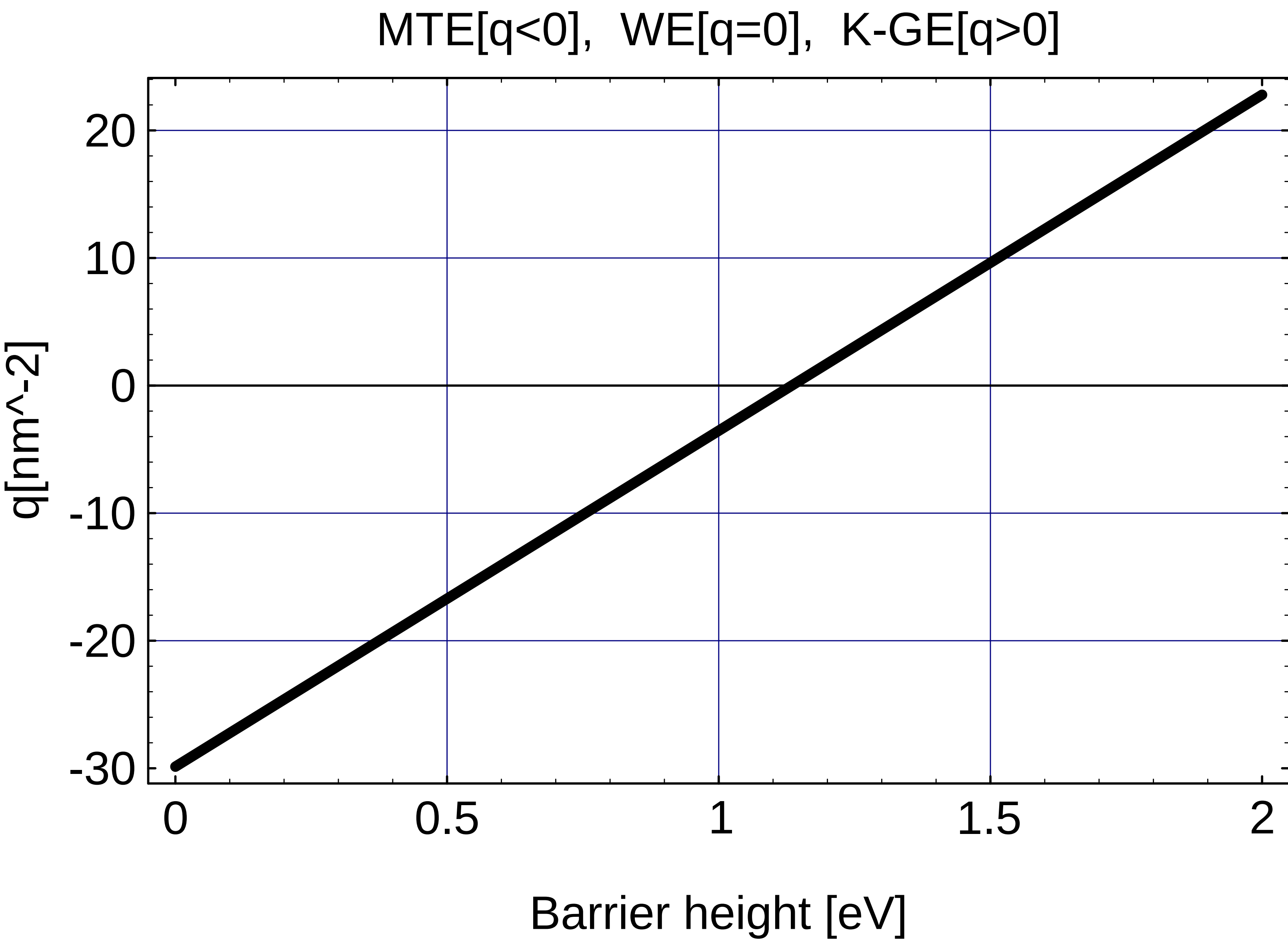
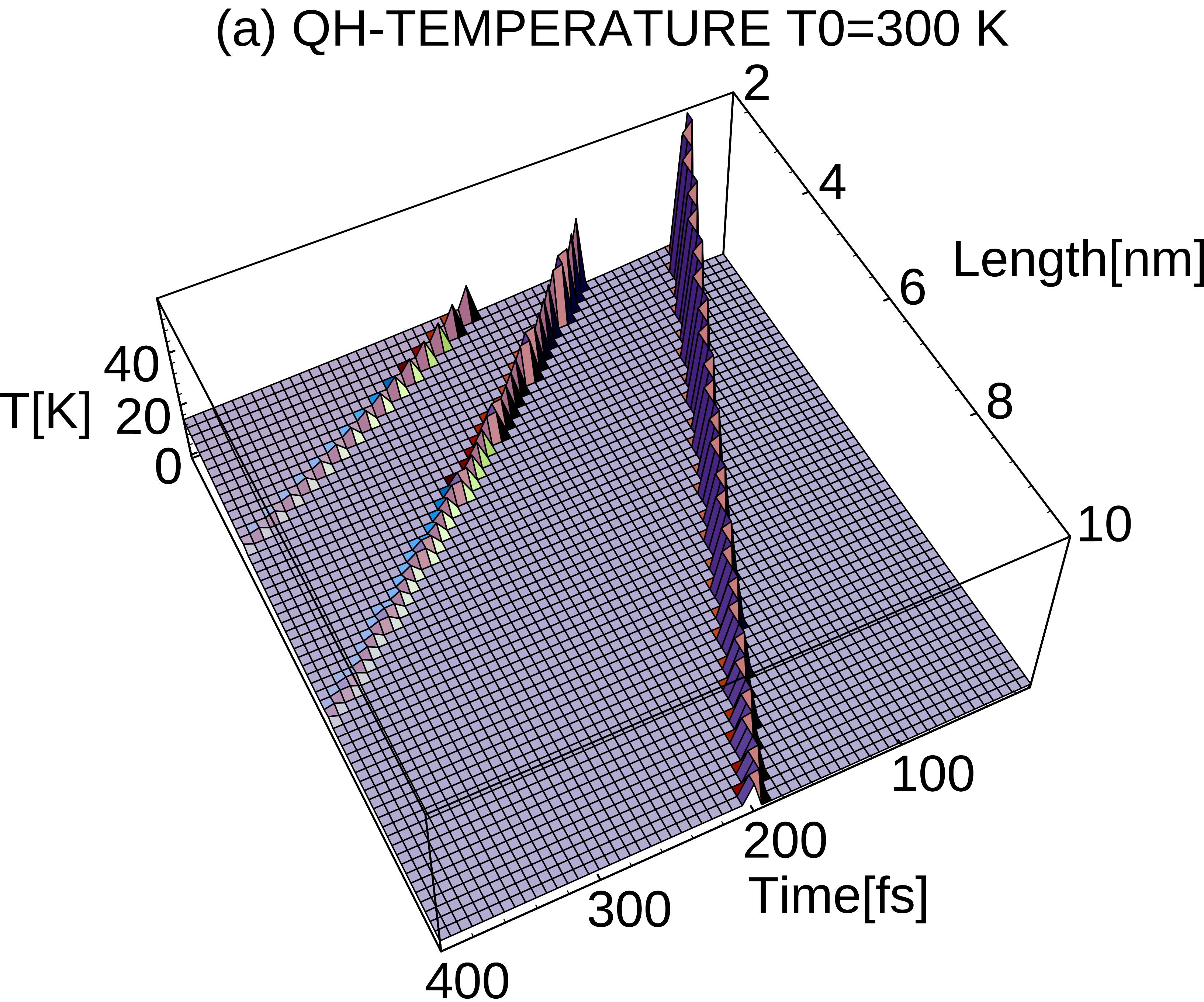
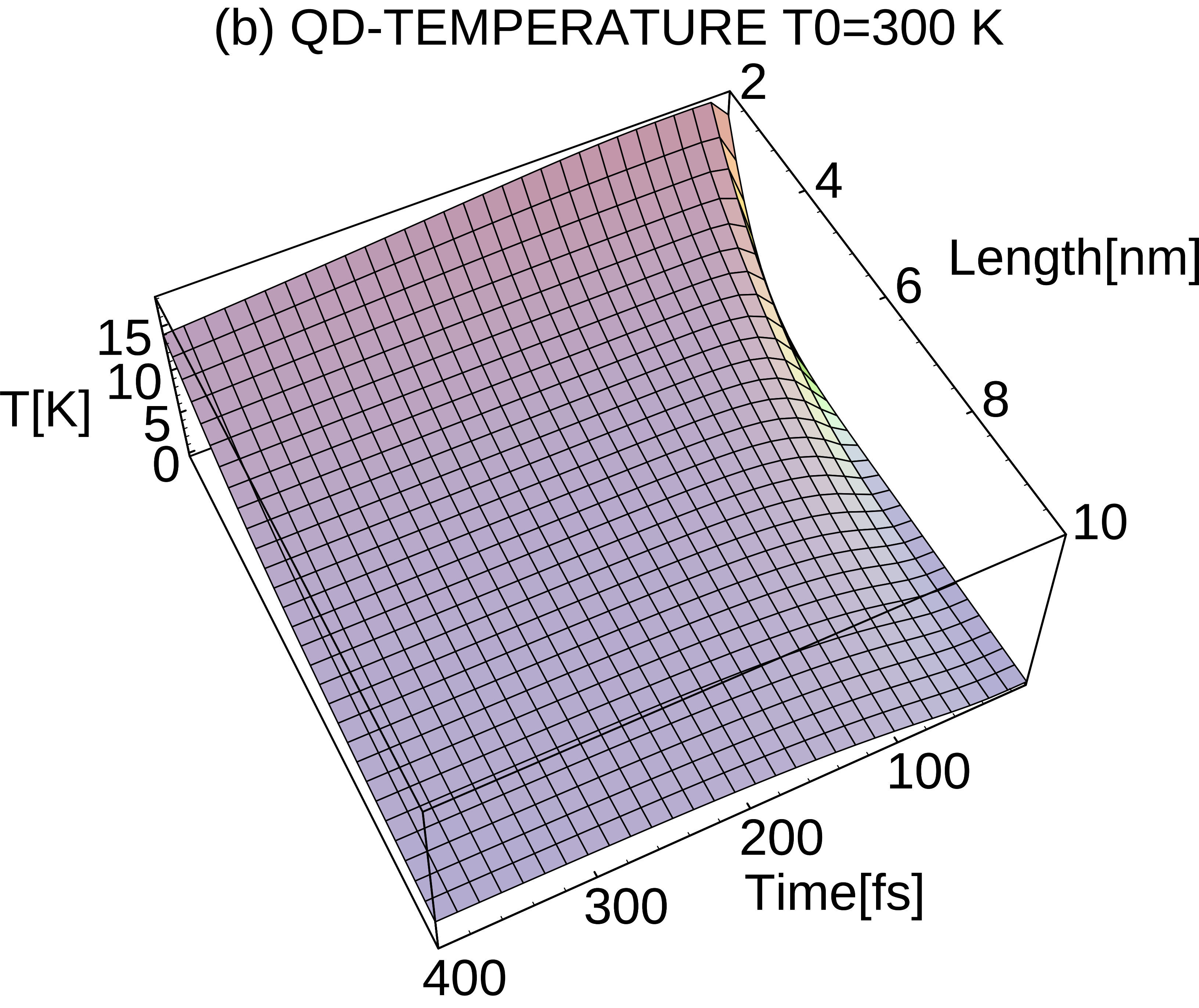


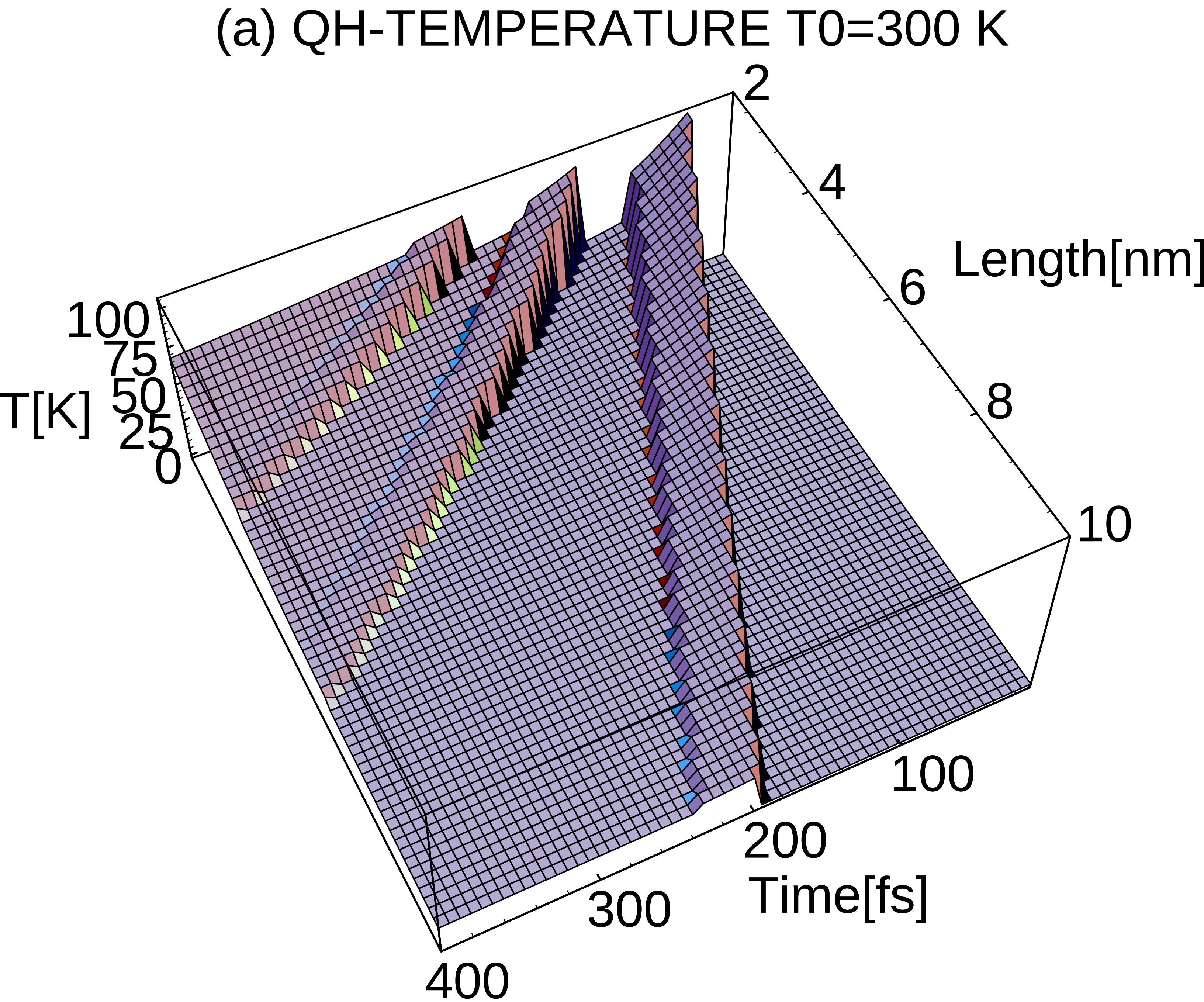
MTE[q<0], WE[q=0], K-GE[q>0]
q[nm^-2]
20
10
0
-10
-20
-30
0
0.5
1
1.5
2
Barrier height [eV]

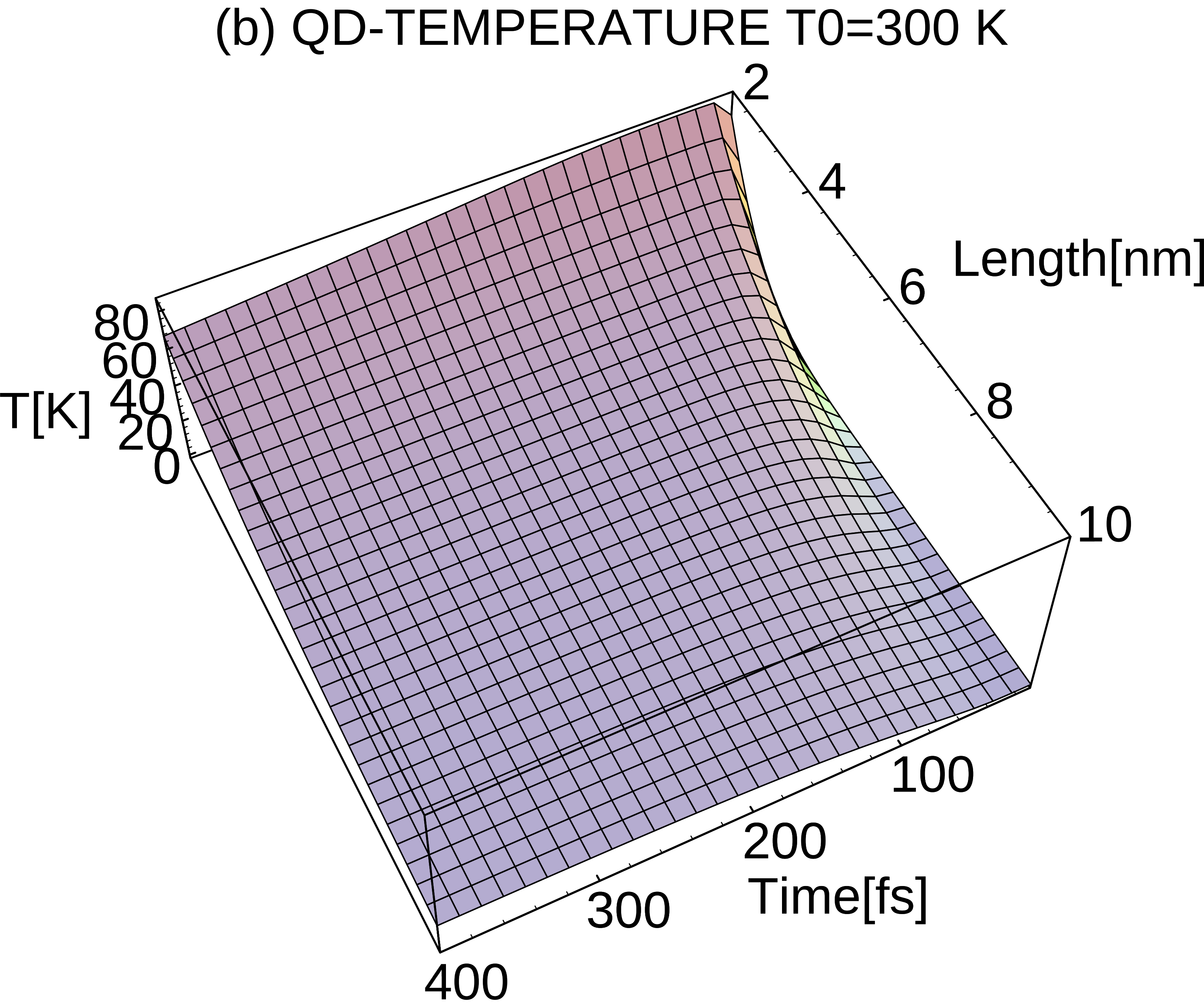


(a) QH-TEMPERATURE T0=300 K
T[K]
0
20
40
2
4
6
8
10
Length[nm]
100
200
300
400
Time[fs]



(b) QD-TEMPERATURE T0=300 K
T[K]
0
5
10
15
Length[nm]
2
4
6
8
10
Time[fs]
100
200
300
400


(a) QH-TEMPERATURE T0=300 K
T[K]
100
75
50
25
0
2
4
6
8
10
Length[nm]
100
200
300
400
Time[fs]


(b) QD-TEMPERATURE T0=300 K
T[K]
0
20
40
60
80
Length[nm]
2
4
6
8
10
Time[fs]
100
200
300
400